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ARTICLE

Application of the Matrix Mechanics Method to Solve the Schrodinger Equation of the Bottomonium System

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Abstract: The matrix mechanics technique [1, 2] was used to analyze the charmonium ($c\bar{c}$ bound state system) in our most recent study [3], and the results showed that it works admirably. In this paper, we attempt to solve the Schrödinger equation for the bottomonium system ($b\bar{b}$ bound state) using the same technique. The results (the masses of the various states and the associated radial wave function) are consistent with experimental and other theoretical results obtained using other methods.

Keywords: Quarkonium, Bottomonium, Non-relativistic potential models, Radial Schrodinger equation.
PACS: 14.40.Pq; 14.65.Fy; 12.39.Jh; 12.39.Pn.

1. Introduction

The term "quarkonium" often refers to a system made up of a heavy quark Q and an antiquark $\bar{Q}$ linked together by a strong interaction. The term "quarkonium" originated from the similarity between the quarkonium system and the positronium system (e^+e^- bound state). The gluon mediates the interaction between quarks just as the photon mediates the electromagnetic interaction between charged particles.

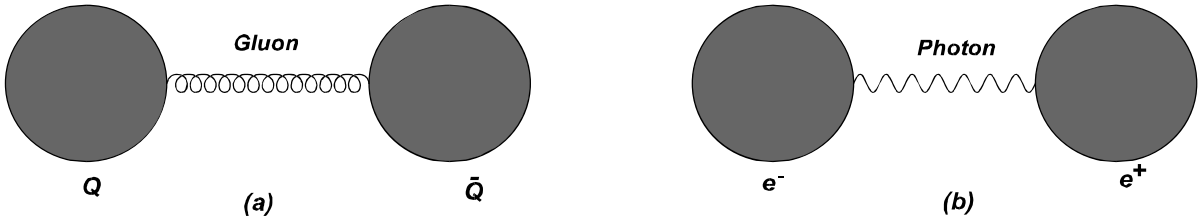

FIG. 1. (a) Strong interaction via one gluon exchange (quarkonium) and (b) electromagnetic interaction via one photon exchange (positronium)

Bottomonium is a quarkonium system made up of a bottom (b) and anti-bottom ($\bar{b}$) quark pair. A team at Fermilab made the first experimental observation of the first bottomonium state Y(1S) (Epsilon) in 1977 [4]. The bottomonium states are produced in hadron colliders such as the Large Hadronic Collider (LHC) and Tevatron, as well as in leptonic colliders like e^+e^- colliders.

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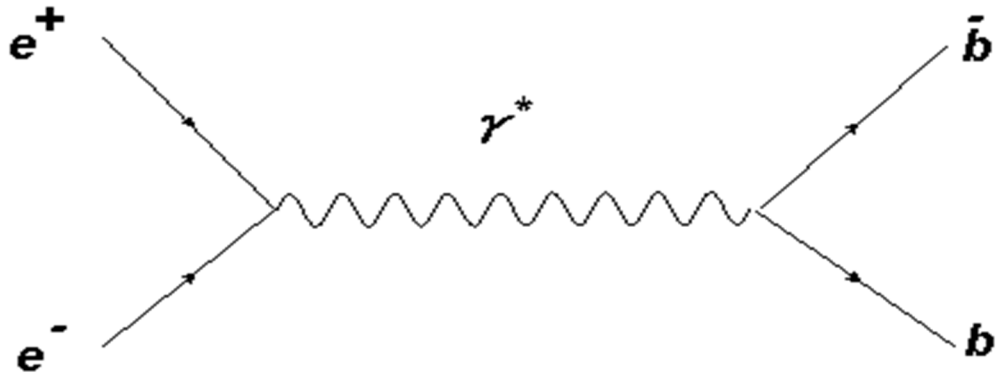

FIG. 2. Example of bottmonium production in an e^+e^- collider.

Because charm and bottom quarks have large masses, it was thought that the bound states of heavy quarks could be characterized by a non-relativistic potential model analogous to positronium [5]. The treatment within the context of non-relativistic quantum mechanics is based on the solution of the Schrödinger equation for the quarkonium system [6]. Numerov algorithm [7], shooting method [8], lattice QCD [9], and the Fourier grid Hamiltonian method [10] are just a few of the numerical methods that have been used to solve this equation. In this work, we use the matrix mechanics method. This method is briefly described in the subsequent section. For further details, see the Refs. [1] and [2].

2. Application of Matrix Mechanics Method to the Radial Schrodinger Equation

In quantum mechanics, the resolution of the equation consists of determining the energy levels and associated eigenfunctions $\psi_{nlm}(r,\theta,\varphi)$. The Hamiltonian exhibits spherical symmetry since the potential solely depends on the separation from the origin. The Schrödinger equation can, therefore, be written in terms of the common spherical coordinate system [11].

$$\Rightarrow \left[-\frac{\hbar^2}{2m}\frac{1}{r}\frac{\partial^2}{\partial r^2}r + \frac{L^2}{2mr^2} + \mathrm{V}(r)\right]\psi_{nlm}(r,\theta,\varphi) = \mathrm{E_n}\psi_{nlm}(r,\theta,\varphi) \quad (1)$$

where:

$$L^2 = -\hbar^2\left[\frac{1}{sin\,\theta}\frac{\partial}{\partial\theta}\left(sin\,\theta\,\frac{\partial}{\partial\theta}\right) + \frac{1}{sin^2\theta}\frac{\partial^2}{\partial\varphi^2}\right] \quad (2)$$

is the modulus squared operator of the orbital angular momentum:

$$\vec{L} = \vec{r}\times\vec{p} = -i\hbar\vec{r}\times\vec{\nabla} \quad (3)$$

The standard approach to solving partial differential equations is the separation of variables. Here, we assume that the wave function is a product of two functions: one dependent on r (the radial part) and the other on θ and φ (the angular part)

$$\psi_{nlm}(r,\theta,\varphi) = R_{nl}(r)Y_l^m(\theta,\varphi) \quad (4)$$

The angular part $Y_l^m(\theta,\varphi)$ (the spherical harmonics) are the eigenfunctions of L^2 and L_z

$$L^2Y_l^m(\theta,\varphi) = \hbar^2 l(l+1)Y_l^m(\theta,\varphi) \quad (5)$$

$$L_z\,Y_l^m(\theta,\varphi) = \hbar m\,Y_l^m(\theta,\varphi) \quad (6)$$

The three-dimensional problem is transformed into a one-dimensional radial equation [11]:

$$-\frac{\hbar^2}{2m}\frac{d^2}{dr^2}\left(rR_{nl}(r)\right) + \left[\frac{\hbar^2 l(l+1)}{2mr^2} + \mathrm{V}(r)\right](rR_{nl}(r)) = \mathrm{E}_n\left(rR_{nl}(r)\right) \quad (7)$$

With $U_{nl}(r) = rR_{nl}(r)$ the equation becomes:

$$-\frac{\hbar^2}{2m}\frac{\mathrm{d}^2U_{nl}(r)}{\mathrm{d}r^2} + \mathrm{V}_{eff}(r)U_{nl}(r) = \mathrm{E}_nU_{nl}(r) \quad (8)$$

where

$$\mathrm{V}_{eff}(r) = \mathrm{V}(r) + \frac{\hbar^2}{2m}\frac{l(l+1)}{r^2} \quad (9)$$

In Ref. [2], it is shown that the matrix mechanic method works perfectly for the problem of the hydrogen atom (a problem with central potential). The matrix mechanics method is based on choosing a simple set of basis states:

$$\psi_n(r) = \sqrt{\frac{2}{a}}\sin\left(\frac{n\pi r}{a}\right) \quad (10)$$

which are simply the eigenfunctions of the infinite potential well with eigenvalues:

$$E_n = \frac{\pi^2\hbar^2n^2}{2ma^2};\ n \geq 1 \quad (11)$$

The corresponding Hamiltonian is given by:

$$H_0 = -\frac{\hbar^2}{2m}\frac{d^2}{r^2} + V_{inf}(r) \quad (12)$$

where:

$$V_{inf}(r) = \begin{cases} 0 \; if \; 0 < r < a \\ +\infty \; otherwise \end{cases} \quad (13)$$

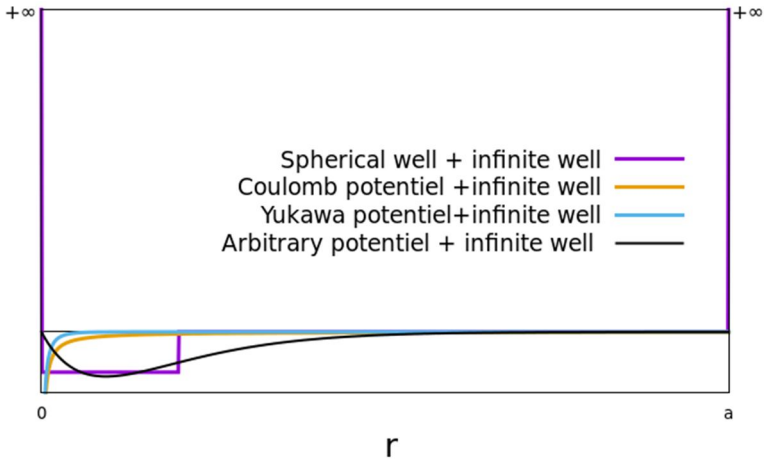

FIG. 3. Examples of potentials plotted along with the infinite square well "embedding" potential of width a.

The infinite well potential model describes a situation where a system is confined or trapped in a certain region. For example, this can represent a gas of molecules inside a container. The model of a particle in a one-dimensional infinite well is a reasonable approximation for an electron moving in a thin metal wire. The potential inside the wire is constant on average but rises sharply at each end.

By embedding the potential of the system in an infinite spherical well of width a, Eq. (8) becomes in the region $0 < r < a$.

$$\left(H_0 + \left[\frac{\hbar^2 l(l+1)}{2mr^2} + \mathrm{V}(r)\right]\right)(U_{nl}(r)) = \mathrm{E}_n U_{nl}(r) \quad (14)$$

The function $\psi_n(r) = \sqrt{\frac{2}{a}}\sin\left(\frac{n\pi r}{a}\right)$ is used to expand the radial function $U(r)$ and to construct the matrix H_{nm} of the Hamiltonian $H = H_0 + V_{eff}(r)$:

$$U(r) = \sum_n c_n \psi_n(r) \quad (15)$$

$$H_{nm} = \langle \psi_n | H | \psi_m \rangle \quad (16)$$

The eigenvalue problem in Eq. (14) becomes now:

$$\sum_{m=1}^{\infty} H_{nm} c_m = E c_n \quad (17)$$

Thus, the problem is transformed from a differential equation to a matrix form problem.

3. Application to the Bottomonium State

The $b\bar{b}$ system interacts via a central potential depending on the relative distance only, $V(|\vec{r}_1 - \vec{r}_2|) = V(r)$. In the center-of-mass system frame, this two-particle system problem is equivalent to a one-particle problem of mass $\mu = m_b/2$ (the reduced mass of the system) subject to the potential $V(r)$. As a consequence of the spherical symmetry, only the resolution of the radial equation is required in this case:

$$-\frac{\hbar^2}{2\mu}\frac{\mathrm{d}^2 U_{nl}(r)}{\mathrm{d}r^2} + \mathrm{V}_{eff}(r) U_{nl}(r) = \mathrm{E}_n U_{nl}(r) \quad (18)$$

Motivated by our results [3] and those of [2], we applied the matrix mechanics method to solve the radial equation of the bottomonium system. In this work, a non-relativistic potential model, known in the literature as the Song-Lin (SL) potential [12], is used:

$$V_{SL}(r) = -\frac{d}{\sqrt{r}} + b\sqrt{r}\,, \quad (19)$$

where d and b are parameters. The potential $V_{SL}(r)$ consists of an attractive Coulomb-like term plus a confining linear term. The Song-Lin potential has been theoretically derived from the fundamental features of Quantum Chromodynamics (QCD) [13]. In [14] and [15], it was pointed out that the SL potential exhibits a number of appealing features that make it a better model than the usual Cornell potential [16, 17]. Other types of potentials, such as the Hulthén-Hellmann potential [19] or the harmonic potential [20], have also been used.

The resolution of the radial Schrödinger equation is carried out following the same strategy used in [2], beginning by constructing the Hamiltonian matrix

H matrix with a specific dimension $n_{\max}$:

$$H_{nm} = \langle\psi_n|H|\psi_m\rangle = \langle\psi_n|H_0|\psi_m\rangle + \langle\psi_n|\mathrm{V}_{eff}(r)|\psi_m\rangle, \quad (20)$$

where the matrix element of H_0 is:

$$\langle\psi_n|H_0|\psi_m\rangle = E_n^0\delta_{nm} = \frac{\pi^2\hbar^2n^2}{2\mu\, a^2}\delta_{nm} \quad (21)$$

and the one of $\mathrm{V}_{eff}(r)$ is expressed by the integral:

$$\langle\psi_n|\mathrm{V}_{eff}(r)|\psi_m\rangle = \frac{2}{a}\int_0^a \sin\left(\frac{n\pi r}{a}\right)\mathrm{V}_{eff}(r)\ \sin\left(\frac{m\pi r}{a}\right)dr \quad (22)$$

Where, in our case:

$$\mathrm{V}_{eff}(r) = V_{SL}(r) + \frac{\hbar^2}{2\,\mu}\frac{l(l+1)}{r^2} \quad (23)$$

is composed of the SL potential term $\boldsymbol{V_{SL}(r)}$ plus the centrifugal term. Using the useful trigonometric relation $\mathbf{\sin(\theta)\sin(\varphi) = \frac{1}{2}(\cos(\theta-\varphi) - \cos(\theta+\varphi))}$ with the change of variable $= \frac{r}{a}$, one can write the integral:

$$\int_0^a \mathbf{\sin\left(\frac{n\pi r}{a}\right)}\mathrm{V}_{\boldsymbol{eff}}(\boldsymbol{r})\ \mathbf{\sin\left(\frac{m\pi r}{a}\right)}\boldsymbol{dr} = \{\boldsymbol{L_1(n+m) - L_1(n-m)}) + \boldsymbol{L_2(n+m) - L_2(n-m)}\} \quad (24)$$

where:

$$L_1(k) = \frac{\hbar^2 l(l+1)}{4\,\mu a}\int_0^1 \frac{(1-\cos(k\pi x)}{x^2}dx \quad (25)$$

$$L_2(k) = \frac{a}{2}\int_0^1 \mathrm{V}_{SL}(ax)(1-\cos(k\pi x)\,dx \quad (26)$$

Once the matrix H of dimension n_{max} x n_{max} is constructed, t is diagonalized to obtain the eigenvalues and the corresponding wavefunctions.

4. Results and Analysis

In this work, we use the same potential parameters as those in Ref. [21]: d = -0.7011 GeV$^{3/2}$ (denoted as "a" in Ref. [21], while "a" n this work refers to the width of the infinite square well), b = 0.8912 GeV$^{1/2}$, and m_b = 4.668 GeV to compare the results. We adopted the natural energy units in the problem, with $\hbar = c = 1$.

We numerically computed the integrals after changing the variable to $x = r/a$. The matrix H was then diagonalized using the Jacobi routine [22] (see the corresponding Fortran code in the Appendix). The mass spectra $M_{b\bar{b}}$ of the bottomonium system are related to the eigenvalue E by the relation: $M_{b\bar{b}} = E + 2m_b$. Table 1 displays the results of our calculation for the mass spectra of the bottomonium system (column 2) using an infinite square well width of a = 5 fermi and n_{max} = 300. The states (first column) are denoted by the spectroscopic notation (nL), where L is the total orbital angular momentum $\vec{L} = \vec{L}_b + \vec{L}_{\bar{b}}$ of the $b\bar{b}$ system. The integer n is the principal quantum number corresponding to the different bottomonium states.

Our results in column 2 are compared with theoretical results in Refs. [21] and [23] (columns 3 and 4), as well as with experimental values (last column). The normalized reduced radial wave functions $U_{nl}(r)$ for different bottomonium states nS (L = 0), nP (L = 1), and nD (L = 2) for n = 1, 2, 3, 4, 5 are illustrated in Figs. 4, 5, and 6, respectively.

TABLE 1. Results of the bottomonium mass spectra (our numbers are rounded to 5 digits)

State nL	Our results	Results of Ref. [21]	Results of Ref. [23]	Experimental results [24]
1S	9.4390	9.444	9.473	9.444
2S	10.095	10.098	10.024	10.023
3S	10.480	10.482	10.327	10.355
4S	10.765	10.766	10.593	10.579
5S	10.997	10.998	10.788	10.865
1P	9.9308	9.930	9.912	9.900
2P	10.359	10.358	10.275	9.900
3P	10.666	10.665	10.580	-------
4P	10.912	10.911	10.703	-------
5P	11.120	11.119	--------	-------
1D	10.235	10.234	10.156	10.161
2D	10.566	10.565	10.434	--------
3D	10.826	10.825	10.625	--------
4D	11.044	11.043	--------	--------
5D	11.233	11.232	--------	--------

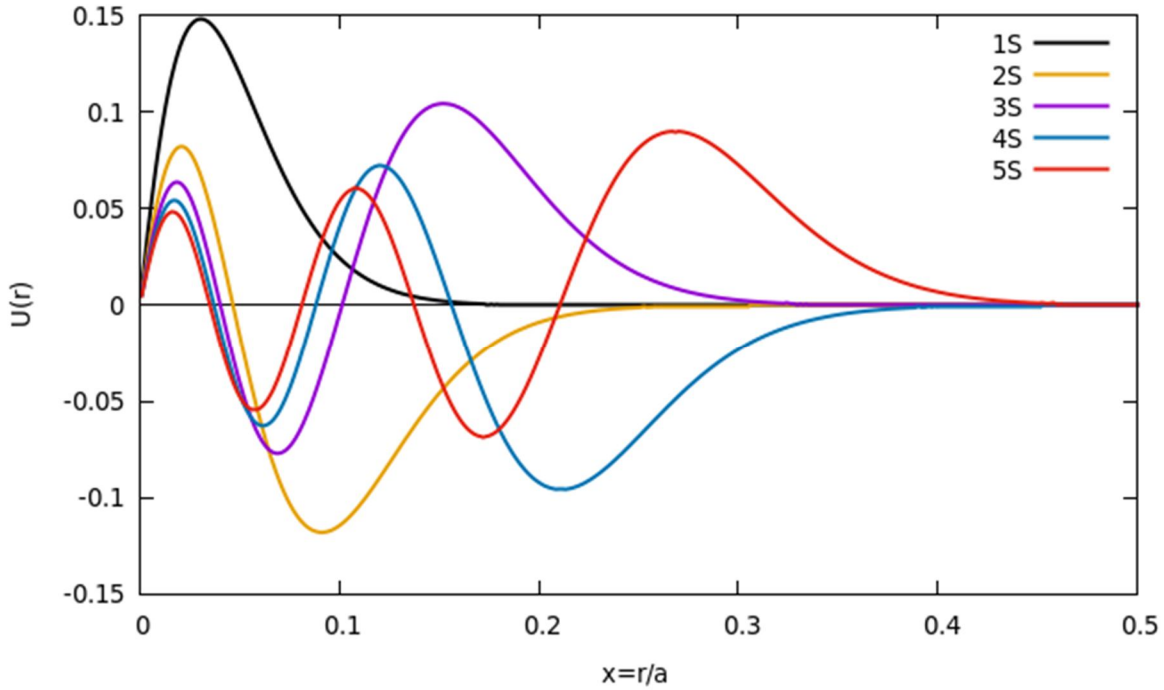

FIG. 4. The normalized reduced radial wave functions for different bottomonium states, nS (L = 0).

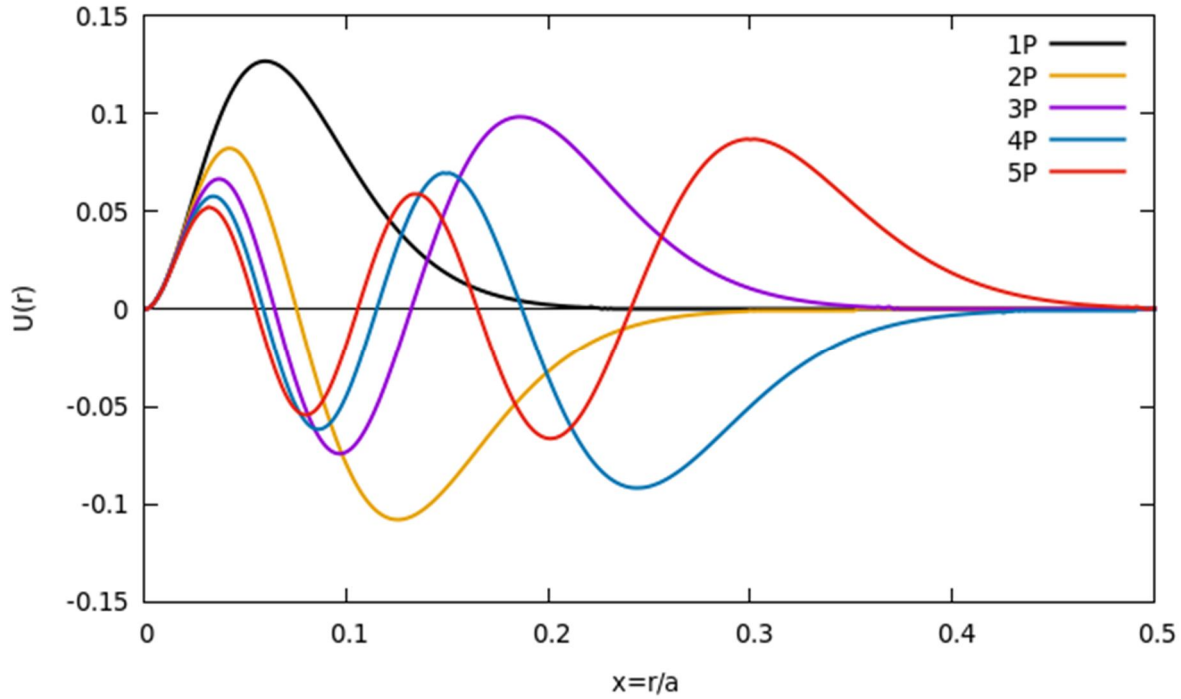

FIG. 5. The normalized reduced radial wave functions for different bottomonium states, nP (L = 1).

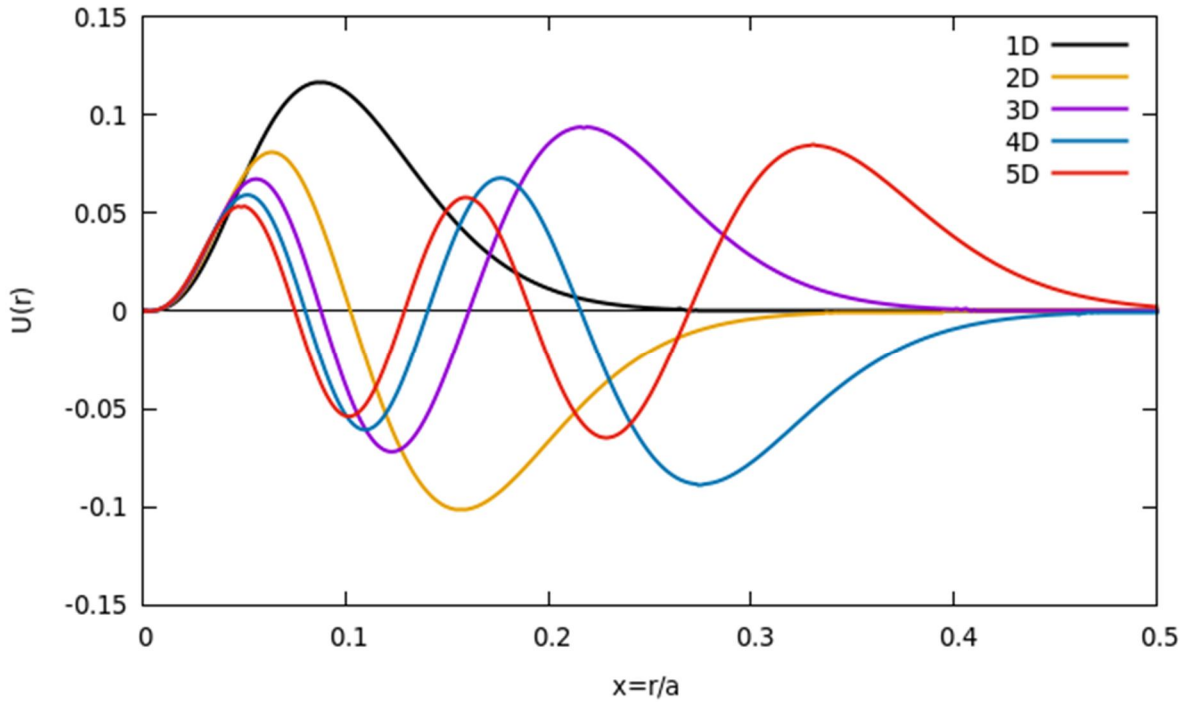

FIG. 6. The normalized reduced radial wave functions for different bottomonium states, nD (L = 2).

5. Conclusion

In the present work, the quarkonium systems have been treated in a non-relativistic framework by solving the corresponding Schrödinger equation. The potential models have a simple form that correctly describes the overall properties of quark-antiquark pairs. Our numerical strategy relies on the matrix mechanics method to compute the full mass spectra and the associated wave functions. This method is based on a specific choice of the basis state vectors in the Hilbert space of the system.

In this paper, we compare our approach with two distinct techniques. We observe that the results are in good agreement with those of [21], where the Numerov method algorithm was used to solve the radial equation, yielding satisfactory agreement with experiments [24]. The agreement is also strong with the results obtained using the asymptotic iteration method [23]. This work serves as the first step toward more complex studies in the near future.

Appendix: Fortran Code

This is the main program of the Fortran code, written in Fortran 90 and compiled with the gfortran compiler under Linux Ubuntu. Lines preceded by "!" are comments intended to clarify the program.

```
IMPLICIT NONE
INTEGER, PARAMETER:: np=300!np should be greater or equal to Nmax
INTEGER:: i,n,m,Nmax,j, nrot,leveln
DOUBLE PRECISION, DIMENSION(np):: d
DOUBLE PRECISION, DIMENSION(0:10000):: x
DOUBLE PRECISION,DIMENSION(np,np):: s1,s3,s4, sum1,sum2 sum3,sum4 DOUBLE PRECISION,DIMENSION(np,np):: delta,integral,a,v
DOUBLE PRECISION:: pi, mb, pas, aa, L1_0, L2_0, L3_0, factor, L
DOUBLE PRECISION:: L1,L2
INTEGER, PARAMETER:: nbrpt=1000 !number of point used in the !integration
COMMON /DATA/aa,pi,mb,L
pi=3.141592653d0
mb=4.668d0 !MASSE OF THE BOTTOM QUARK
! INPUTS Nmax: H DIMENSION, aa: VALUE OF THE DEPTH a IN FERMI,
!L: ORBITAL MOMENTUM,
READ(*,*) Nmax,aa,L
factor=5.076142132d0 !CONVERSION FACTOR: from fermi to Gev-1 unit
aa=factor*aa ! aa=a the VALUE OF THE DEPTH OF THE INFINITE SQUARE WELL
! STARTING CONTRUCTING Hnm
DO n=1,Nmax
DO m=1,Nmax
IF(n/=m) THEN
```

```
delta(n,m)=0.0d0
ELSE
delta(n,m)=(pi*n/aa)**2/mb +2*mb ! E^0 +2mb
END IF
!COMPUTATION OF THE INTEGRANDS AT THE PROBLEMATIC POINT r=0
x(0)=0.0d0
pas=1.d0/nbrpt
x(1)=0.0d0+pas
L2_0=0.0d0
L1_0=2*n*m*pi**2/(mb*aa)
L3_0=0.d0
s1(n,m)=s1(n,m)+(L2(x(1),n+m)+L2_0)*pas/2.
s2(n,m)=s2(n,m)+(L2(x(1),n-m)+L2_0)*pas/2.
s3(n,m)=s3(n,m)+(L1(x(1),n+m)+L1_0)*pas/2.
s4(n,m)=s4(n,m)+(L1(x(1),n-m)+L1_0)*pas/2.
s5(n,m)=s5(n,m)+(L3(x(1),n+m)+L3_0)*pas/2.
s6(n,m)=s6(n,m)+(L3(x(1),n-m)+L3_0)*pas/2.
!STARTING INTEGRATION FROM x(2) to x(n)=1
DO i=2,nbrpt
x(i)=x(0)+i*pas
!CENTRIFUGAL TERM
s1(n,m)=s1(n,m)+(L1(x(i),n+m)+L1(x(i-
1),n+m))*pas/2.
s2(n,m)=s2(n,m)+(L1(x(i),n-m)+L1(x(i-1),n-
m))*pas/2.
!COULOMB LIKE ATTRACTIVE TERM + LINEAR TERM (SL potential)
s3(n,m)=s3(n,m)+(L2(x(i),n+m)+L2(x(i-
1),n+m))*pas/2.
s4(n,m)=s4(n,m)+(L2(x(i),n-m)+L2(x(i-1),n-
m))*pas/2.
END DO
END DO
END DO
!COMPUTING Li(n+m)-Li(n-m) i=1,2
sum1=s1-s2
sum2=s3-s4
!COMPUTING {L1(n+m)-L1(n-m)}+{L2(n+m)-L2(n-m)}
integral=(2./aa)*(sum1+sum2)
!HAMILTONIAN MATRIX a(n,m)=H(n,m)
a=delta+integral
!DIAGONALIZATION
n=Nmax
CALL jacobi(a,n,np,d,v,nrot)
CALL eigsrt(d,v,n,np)
! NOMBER OF THE LEVELS TO PRINT THE MASS VALUE
nlevel=5
DO j=0, nlevel
WRITE(*,*) 'level', j,' ', 'mass', d(nmax-j)
ENDDO
END
! STARTING COMPUTING THE VALUES OF THE RADIALE FUNCTION U(R)
open(3,file='values_of_u1_0.txt',status='new')
open(4,file='values_of _u2_0.txt',status='new')
open(5,file='values_of _u3_0.txt',status='new')
open(6,file='values_of _u4_0.txt',status='new')
open(7,file='values_of _u5_0.txt',status='new')
do i=1,nbrpt
u(1,i)=0.d0
u(2,i)=0.d0
u(3,i)=0.d0
u(4,i)=0.d0
u(5,i)=0.d0
do m=1,Nmax
u(1,i)=u(1,i)+dsqrt(2.d0)*dsin(m*pi*x(i))*v(m,n
max)
u(2,i)=u(2,i)+dsqrt(2.d0)*dsin(m*pi*x(i))*v(m,n
max-1)
u(3,i)=u(3,i)+sqrt(2.d0)*dsin(m*pi*x(i))*v(m,n
max-2)
u(4,i)=u(4,i)+dsqrt(2.d0)*dsin(m*pi*x(i))*v(m,n
max-3)
u(5,i)=u(5,i)+sqrt(2.d0)*dsin(m*pi*x(i))*v(m,n
max-4)
enddo
enddo
norme1=0.d0
norme2=0.d0
norme3=0.d0
norme4=0.d0
norme5=0.d0
do i=1,nbrpt
norme1=norme1+u(1,i)**2
norme2=norme2+u(2,i)**2
norme3=norme3+u(3,i)**2
norme4=norme4+u(4,i)**2
norme5=norme5+u(5,i)**2
enddo
do i=1,nbrpt
write(3,*) x(i),u(1,i)/dsqrt(norme1)
write(4,*) x(i),u(2,i)/dsqrt(norme2)
write(5,*) x(i),u(3,i)/dsqrt(norme3)
write(6,*) x(i),u(4,i)/dsqrt(norme4)
write(7,*) x(i),u(5,i)/dsqrt(norme5)
enddo
! THIS FUNCTION COMPUTES THE INTEGRAND OF THE CENTRIFUGAL TERM
DOUBLE PRECISION FUNCTION L1(x,k)
INTEGER k
DOUBLE PRECISION pi,aa,mb,x,L
COMMON /DATA/aa,pi,mb,L
L1=(l*(l+1)/mb)*(1-dcos(k*pi*x))/(2.*aa*x**2)
RETURN
```

```
END FUNCTION
! THIS FUNCTION COMPUTES THE INTEGRAND OF THE COULOMBIEN LIKE !TERM+LINEAR CONFINING TERM (SL POTENTIEL)
DOUBLE PRECISION FUNCTION L2(x,k)
INTEGER k
DOUBLE PRECISION x,pi,mb,aa,b,L
COMMON /DATA/aa,pi,mb,L
a1=-0.7011d0
b=0.8912d0
L2=(1-
dcos(k*pi*x))*(a1*dsqrt(aa)/dsqrt(x)+(aa*dsqrt(
aa))*b*dsqrt(x))/2
RETURN
END FUNCTION
```

6. Acknowledgments

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